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MULTIDIMENSIONAL QUADRATURE FORMULAS USING PARTIAL DERIVATES.(U)

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MULTIDIMENSIONAL QUADRATURE FORMULAS USING PARTIAL DERIVATIVES

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Conventional multidimensional quadrature formula employ a weighted sum of function values to approximate a multiple integral over a hyperrectangle. This paper considers the problem of enhancing the traditional formulas by the addition of certain partial derivative correction terms evaluated on the boundary of the domain of integration. Numerical results for double and triple integrals indicate the formulas of degrees of precision 3 and precision 5 are both accurate and efficient.

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PREFACE

A recent report, based on a dissertation prepared by the first author, addressed the problem of enhancing the accuracy of traditional cubature formulas for evaluating double integrals numerically over rectangles by the addition of first- and mixed second-order partial derivative correction terms evaluated on the boundary of the domain of integration.

The present report, based on a paper presented at the Society for Industrial and Applied Mathematics (SIAM) 1977 Fall meeting, 31 October to 2 November, Albuquerque, New Mexico, generalizes the results of the dissertation to multidimensional integrals over hyperrectangles. In addition, 53 new multidimensional quadrature formulas with boundary partial derivative correction terms are given. Numerical results are presented for double and triple integrals.

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for J. H. FOXGROVER, RADM, USN
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MULTIDIMENSIONAL QUADRATURE FORMULAS USING PARTIAL DERIVATIVES

WAYNE E. HOOVER[1] AND J. SUTHERLAND FRAME[2]

I. INTRODUCTION

Traditional methods of approximating multidimensional integrals of the form

$$I(f) = \int_{a_N}^{b_N} \cdots \int_{a_1}^{b_1} f(x_1, \ldots, x_N)dx_1 \cdots dx_N$$

over the hyperrectangle

$$R = \prod_{i=1}^{N} \left[a_i, b_i\right], \quad a_i, b_i \text{ real},$$

employ a weighted sum of function values

$$Q(f) = \sum_{i=1}^{N} w_i f(x_{i1}, \ldots, x_{iN}).$$

The w_i are called weights and the $(x_{i1}, \ldots, x_{iN})$ are called nodes. The difference

$$E(f) = I(f) - Q(f)$$

is the truncation error (or error).

Let $p_k = p_k(x_1, \ldots, x_N)$ be a polynomial of degree k in N variables. Then the multidimensional quadrature formula or rule Q(f) is said to be of order k or have degree of precision k if for any p_k, $E(p_k) = 0$, but $E(p_{k+1}) \neq 0$ for at least one polynomial p_{k+1}.

Since it is not uncommon for numerical procedures to make use of partial derivatives, e.g., in optimization techniques, it is surprising that very little seems to be known concerning the use of partial derivatives in nonproduct multidimensional quadrature rules. Stroud [21] gives only one cubature formula, C_2:2-1, due to Ionescue [11], which uses partial derivatives of the integrand.

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Therefore, the objective of this investigation is to construct a number of new composite multidimensional quadrature formulas of orders 3 and 5 using first- and mixed second-order partial derivative correction terms in addition to function values of the integrand. Numerical results indicate that the use of partial derivatives evaluated on the boundary of R increases the accuracy and efficiency of composite multidimensional integration formulas. The efficiency of the composite formulations may be explained in terms of the following three properties.

First, consider an m-point rule in which all the nodes lie in the interior of R. When R is partitioned into s subhyperrectangles or cells and the rule is applied to each cell, the total number of nodes is ms since the nodes are interior to each cell. A more efficient procedure is to employ an integration rule in which some nodes coincide with the boundary of the domain of integration. Then when the domain is subdivided, these nodes are included in more than one cell. Thus the total number of nodes is considerably less than the sum of their numbers in each cell. This we call the "inclusion property."

The second property is known as "persistence of form." Briefly, this means that for some functions it requires approximately the same if not less computer time to evaluate a partial derivative as it does the function since the form of a partial derivative follows that of the function. Thus, part of the calculation required for the function may be reused for the partial derivative evaluation. Further computer economy can also be achieved if the partial derivative is evaluated at the same point as the function since only one calculation of the location of the point is required.

Finally, efficiency results from applying the "alternating sign property." Essentially this means that in the composite formulation of a rule, the weights assigned to the partial derivative nodes, equal in magnitude but opposite in sign, cancel at interior points and consequently, the partials need be evaluated only on the boundary of R.

In Section III, the method of undetermined coefficients in conjunction with the inclusion property, the persistence of form property, and the alternating sign property is employed to construct a number of new partial derivative corrected multidimensional numerical integration formulas.

To conclude this section, observe that because of the "boundary effect," that is, most of the volume of a hyperrectangle lies near the boundary, it seems natural to construct multidimensional quadrature rules with boundary partial derivative correction terms. Indeed, for the hyperrectangle R with edge $w_k = b_k - a_k$, the set of points whose distance from some edge is less than or equal $\epsilon/2$ has volume

$$\prod_{k=1}^{N} w_k - \prod_{k=1}^{N} (w_k - \epsilon w_k) = \left[1-(1-\epsilon)^N\right] \prod_{k=1}^{N} w_k$$

which approaches the volume of R as the number of dimensions, N, approaches infinity. For example, the volume of the set of points whose distance from some edge of a 100-dimensional hyperrectangle, R, is less than or equal 0.05 is 99.997% the volume of R.

II. THE ALTERNATING SIGN PROPERTY

In this section, several observations will be made for the specific case $N = 2$.

A study of the Euler-Maclaurin Summation formula for a function of two variables suggests the possibility of constructing nonproduct cubature formulas involving first- and perhaps mixed second-order partial derivative correction terms with weights of equal magnitude but alternate signs at the four corners or at the midpoints of the sides of the rectangular domain of integration, $R = [-h_1, h_1] \times [-h_2, h_2]$, so that when the rule is compounded or repeated, the weights cancel except on the boundary. As previously noted, this is called the alternating sign property. See Figure 1.

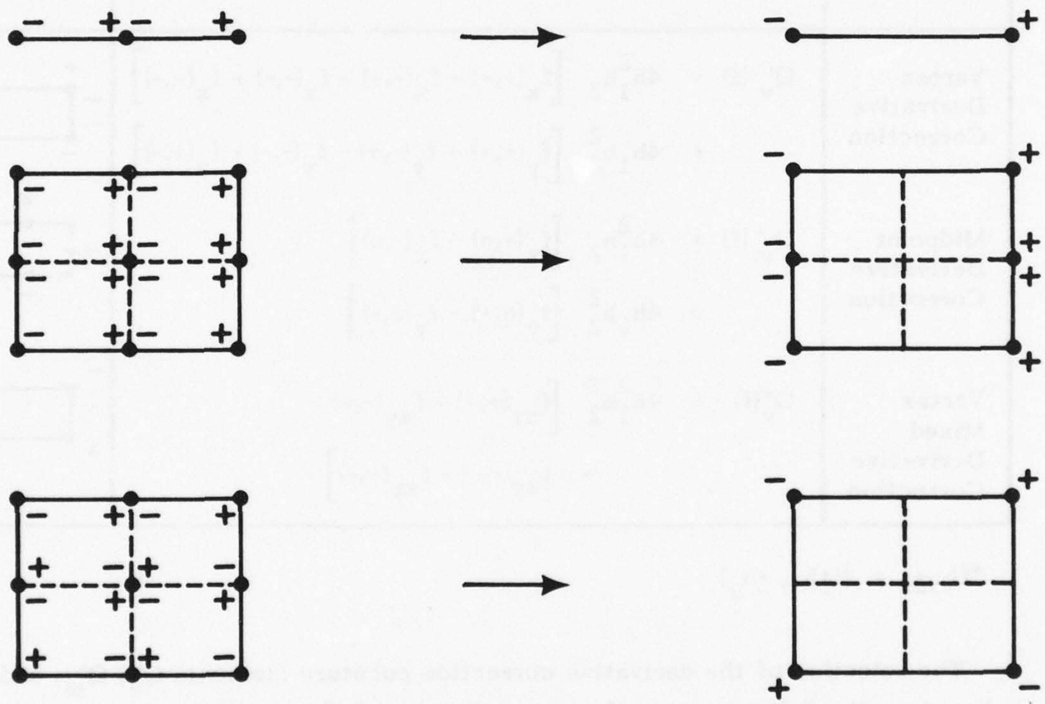
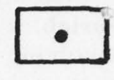
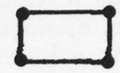
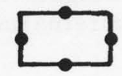
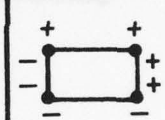
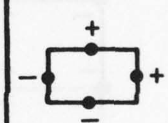
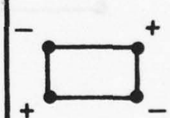


Figure 1
Alternating Sign Property for N = 1 and 2

This investigation will consider the six "cubature elements" listed in Table I.

Table I

Cubature Elements

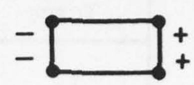
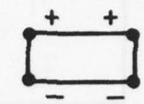
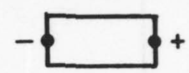
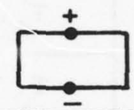
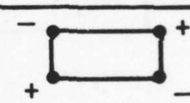
Name	Cubature Element	Diagram
Centroid Value	$Q_c(f) = 4h_1h_2f(o, o)$	
Vertex Sum	$Q_v(f) = 4h_1h_2\left[f(+,+)^* + f(-,+) + f(-,-) + f(+,-)\right]$	
Midpoint Sum	$Q_m(f) = 4h_1h_2\left[f(+,o) + f(o,+) + f(-,o) + f(o,-)\right]$	
Vertex Derivative Correction	$Q'_v(f) = 4h_1^2h_2\left[f_x(+,+) - f_x(-,+) - f_x(-,-) + f_x(+,-)\right]$ $+\ 4h_1h_2^2\left[f_y(+,+) + f_y(-,+) - f_y(-,-) - f_y(+,-)\right]$	
Midpoint Derivative Correction	$Q'_m(f) = 4h_1^2h_2\left[f_x(+,o) - f_x(-,o)\right]$ $+\ 4h_1h_2^2\left[f_y(o,+) - f_y(o,-)\right]$	
Vertex Mixed Derivative Correction	$Q''_v(f) = 4h_1^2h_2^2\left[f_{xy}(+,+) - f_{xy}(-,+)\right.$ $\left.+\ f_{xy}(-,-) - f_{xy}(+,-)\right]$	

$^*f(\pm,\pm) = f(\pm h_1, \pm h_2)$

The selection of the derivative correction cubature elements Q'_v, Q'_m, and Q''_v is based on the following considerations. For α and β nonnegative integers, define the partial derivative correction terms, T_i, listed in Table II.

Table II

Partial Derivative Correction Terms

Name	Correction Term	Diagram
T_1	$\mathscr{D}_2^\beta \mathscr{D}_1^\alpha \left[f(+,+)^* - f(-,+) - f(-,-) + f(+,-)\right]$	
T_2	$\mathscr{D}_2^\beta \mathscr{D}_1^\alpha \left[f(+,+) + f(-,+) - f(-,-) - f(+,-)\right]$	
T_3	$\mathscr{D}_2^\beta \mathscr{D}_1^\alpha \left[f(+,o) - f(-,o)\right]$	
T_4	$\mathscr{D}_2^\beta \mathscr{D}_1^\alpha \left[f(0,+) - f(o,-)\right]$	
T_5	$\mathscr{D}_2^\beta \mathscr{D}_1^\alpha \left[f(+,+) - f(-,+) + f(-,-) - f(+,-)\right]$	

$^*f(\pm,\pm) = f(\pm h_1, \pm h_2)$

Now suppose $f(x_1,x_2)$ can be expanded in a Taylor series about the point (0,0) as far as may be required. If the series converges on R, then the correction terms assume zero or nonzero values as indicated in Table III. Examination of Table III shows the odd/even constraints which must be placed upon α and β in order to avoid nonzero correction terms, T_i, the components of the partial derivative correction elements Q'_v, Q'_m, and Q''_v. These cubature elements are then candidates for inclusion in cubature formulas. In Section VI, the n-dimensional generalizations of the elements are used as building blocks to construct 53 new multidimensional quadrature rules with partial derivative correction terms. The results are summarized in Table VII.

Table III

Values of the Correction Terms

Correction Term	α Even β Even	α Odd β Even	α Even β Odd	α Odd β Odd
T_1	0	Nonzero	0	0
T_2	0	0	Nonzero	0
T_3	0	Nonzero	0	0
T_4	0	0	Nonzero	0
T_5	0	0	0	Nonzero

III. DERIVATION OF MINTOV

Denote the center of the hyperrectangle

$$R = \prod_{j=1}^{N} \left[-h_j, h_j\right]$$

by $c = (0,\ldots,0)$, the 2^N vertices by $v = (v_1, \ldots, v_N)$ where $v_j = h_j$ or $-h_j$, the 2N midpoints of the bounding (N-1)-dimensional hyperrectangles or "sides" of R by $m = (m_1, \ldots, m_N)$ where $m_j = h_j$ or $-h_j$ and $m_i = 0$ for $i \neq j$, and the volume by

$$h = \prod_{j=1}^{N} 2h_j .$$

For $p = m$ or v, define the sign functionals

$$\sigma_j(p) = \begin{cases} -1 \text{ if } p_j = -h_j \\ +1 \text{ otherwise} \end{cases} \qquad (1)$$

$$\sigma_{jk}(p) = \sigma_j(p)\, \sigma_k(p)$$

and the first- and second-order partial derivative correction terms

$$
\begin{aligned}
D_j f(p) &= \sum_p \sigma_j(p) \mathcal{D}'_j f(p) \\
D_{jk} f(v) &= \sum_c \sigma_{jk}(v) \mathcal{D}'_k \mathcal{D}'_j f(v)
\end{aligned}
\tag{2}
$$

where the sums are over the indicated points and

$$\mathcal{D}^{\alpha}_j f(x) = \frac{\partial^{\alpha}}{\partial x_j^{\alpha}} f(x_1, \ldots, x_N)$$

denotes the α-th partial derivative of f(x) with respect to the j-th variable. Figures 2 and 3 illustrate two of the partial derivative correction terms for the 4-cube. Careful inspection will reveal the sign arrangements of $D_1 f(v)$ and $D_{12} f(v)$ for the 2- and 3- cubes.

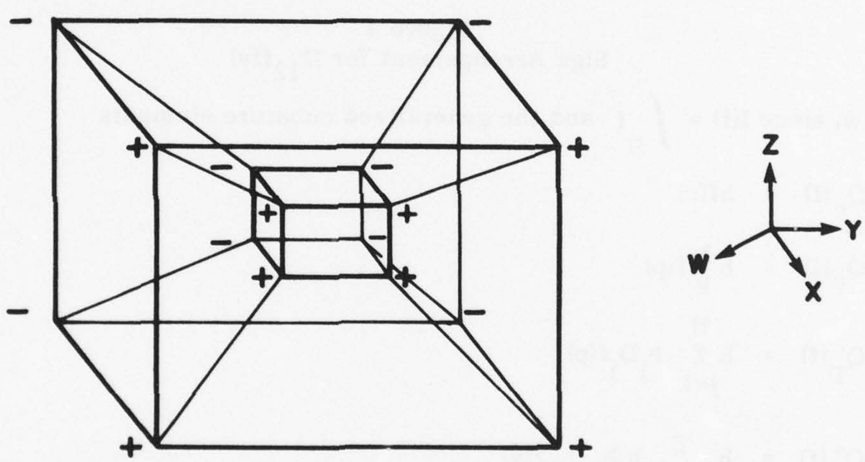


Figure 2
Sign Arrangement for $D_1 f(v)$

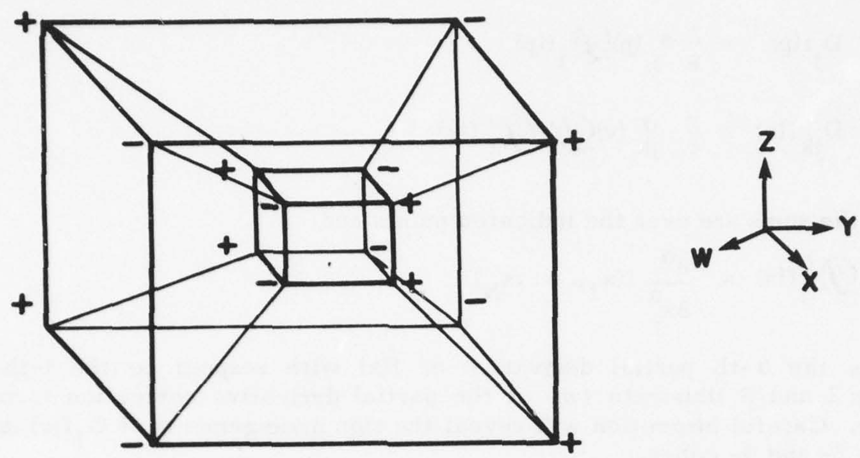


Figure 3
Sign Arrangement for $D_{12}f(v)$

Now, since $I(f) = \int_R f$ and the generalized cubature elements

$$
\begin{aligned}
Q_c(f) &= hf(c) \\
Q_p(f) &= h \sum_p f(p) \\
Q'_p(f) &= h \sum_{j=1}^{N} h_j D_j f(p) \\
Q''_v(f) &= h \sum_{j<k} h_j h_k D_{jk} f(v)
\end{aligned}
\qquad (3)
$$

vanish for functions which are odd in any variable, we may approximate I(f) by the linear combination

$$I(f) \approx Q(f) = \lambda_1 Q_c + \lambda_2 Q_v + \lambda_3 Q'_v + \lambda_4 Q''_v \qquad (4)$$

which is exact for the even functions 1, x_1^2, x_1^4, $x_1^2 x_2^2$, x_1^6, $x_1^4 x_2^2$, and $x_1^2 x_2^2 x_3^2$. By symmetry then, Q(f) will also be exact for all polynomials of degree at most 5.

<u>THEOREM.</u> If f(x) has continuous partial derivatives of the first six orders on

$$R = \prod_{j=1}^{N} \left[-h_j, h_j\right], \text{ then}$$

$$I(f) = \left[8Q_c + (7Q_v - Q'_v - Q''_v/3)/2^N\right]/15 + E(f) \tag{5}$$

is a multidimensional quadrature formula with degree of precision 5. The truncation error, E(f), is bounded by

$$|E(f)| \leq h \left[E_6 + 35E_{42} + 280E_{222}\right]/9450 \tag{6}$$

where

$$M^{\alpha\beta\ldots\gamma}_{jk\ldots L} = \max \left| \mathcal{D}^{\gamma}_{L} \cdots \mathcal{D}^{\beta}_{k} \mathcal{D}^{\alpha}_{j} f(x) \right|$$

$$E_{\alpha} = \sum_{j=1}^{N} h_j^{\alpha} M_j^{\alpha}$$

$$E_{\alpha\beta} = \sum_{\substack{j,\,k=1 \\ j \neq k}}^{N} h_j^{\alpha} h_k^{\beta} M_{jk}^{\alpha\beta} \tag{7}$$

$$E_{\alpha\beta\gamma} = \sum_{j<k<L} h_j^{\alpha} h_k^{\beta} h_1 M_{jkL}^{\alpha\beta\gamma} .$$

<u>PROOF.</u> By applying Taylor's theorem for N-variables to (4) and equating coefficients of similar terms, one obtains the linear system

$$\begin{bmatrix} 1 & 2^N & 0 & 0 \\ 0 & 2^{N-1} & 2^N & 0 \\ 0 & \frac{1}{3}\,2^{N-3} & \frac{1}{3}\,2^{N-1} & 0 \\ 0 & 2^{N-2} & 2^N & 2^N \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \\ \lambda_4 \end{bmatrix} = \begin{bmatrix} 1 \\ \frac{1}{6} \\ \frac{1}{120} \\ \frac{1}{36} \end{bmatrix} \tag{8}$$

having the unique solution

$$(\lambda_1, \lambda_2, \lambda_3, \lambda_4) = \left(\frac{8}{15}, \frac{7}{2^N 15}, \frac{-1}{2^N 15}, \frac{-1}{2^N 45}\right). \tag{9}$$

The bound (6) on the truncation error is a consequence of Taylor's theorem and is a straightforward calculation. Observe that the last term in the error bound appears only for $N > 2$.

The name MINTOV (for Multiple INTegration, Order 5) is given to (5).

IV. COMPOSITE FORMULATION OF MINTOV

In order to obtain the composite formulation of (5) for an arbitrary hyperrectangle

$$R = \prod_{i=1}^{N} \left[a_i, b_i\right],$$

partition each interval $\left[a_i, b_i\right]$ into n_j subintervals each of length $h_j = w_j/n_j$ where $w_j = b_j - a_j$. Denote the volume of each cell thus obtained by

$$h = \prod_{j=1}^{N} h_j$$

and the volume of R by

$$w = \prod_{j=1}^{N} w_j .$$

To condense notation, define

$$\begin{aligned}
\zeta(\Theta) &= (a_1+h_1(i_1-\Theta), \ldots, a_N+h_N(i_N-\Theta)) \\
\zeta(x_j,\Theta) &= (a_1+h_1(i_1-\Theta), \ldots, x_j, a_{j+1}+h_{j+1}(i_{j+1}-\Theta), \ldots, \\
&\quad a_N+h_N(i_N-\Theta)) \qquad (10) \\
\xi(x_j) &= (a_1+i_1h_1, \ldots, x_j, a_{j+1}+i_{j+1}h_{j+1}, \ldots, a_N+i_Nh_N)
\end{aligned}$$

$$\xi(x_j, x_k) = (a_1 + i_1 h_1, \ldots, x_j, a_{j+1} + i_{j+1} h_{j+1}, \ldots x_k, a_{k+1} + i_{k+1} h_{k+1}, \ldots, a_N + i_N h_N)$$

and

$$\sum_{\alpha=1}^{N} \bullet \sum_{i_\alpha=1}^{n_\alpha} = \sum_{i_N=1}^{n_N} \cdots \sum_{i_2=1}^{n_2} \sum_{i_1=1}^{n_1} \cdot$$

Furthermore,

$$A_c = h \sum_{\alpha=1}^{N} \bullet \sum_{i_\alpha=1}^{n_\alpha} f[\zeta(½)]$$

$$A_v = h \sum_{\alpha=1}^{N} \bullet \sum_{i_\alpha=0}^{n_\alpha} \gamma f[\zeta(0)] \tag{11}$$

$$A_m = h \sum_{j=1}^{N} \sum_{\alpha=1}^{N} \bullet \sum_{i_\alpha=\tau_\alpha}^{n_\alpha} \gamma f[\zeta(a_j + i_j h_j, ½)] \qquad \tau_\alpha = \begin{cases} 0 \text{ if } \alpha = j \\ 1 \quad \alpha \neq j \end{cases}$$

$$A'_v = h \sum_{j=1}^{N} \sum_{\substack{\alpha=1 \\ \alpha \neq j}}^{N} \bullet \sum_{i_\alpha=0}^{n_\alpha} \gamma h_j \mathcal{D}'_j [f(\xi(b_j)) - f(\xi(a_j))]$$

$$A'_m = h \sum_{j=1}^{N} \sum_{\substack{\alpha=1 \\ \alpha \neq j}}^{N} \bullet \sum_{i_\alpha=1}^{n_\alpha} h_j \mathcal{D}'_j [f(\zeta(b_j, ½)) - f(\zeta(a_j, ½))]$$

$$A''_v = h \sum_{j<k} \sum_{\substack{\alpha=1 \\ \alpha \neq j,k}}^{N} \bullet \sum_{i_\alpha=0}^{n_\alpha} \gamma h_j h_k \mathcal{D}'_k \mathcal{D}'_j [f(\xi(a_j, a_k)) - f(\xi(a_j, b_k)) - f(\xi(b_j, a_k)) + f(\xi(b_j, b_k))].$$

Observe that the weight γ is to be assigned when the node is common to γ cells.

COROLLARY. If f(x) has continuous partial derivatives of the first six orders on the hyperrectangle R, then

$$\int_{a_N}^{b_N} \cdots \int_{a_1}^{b_1} f(x_1, \ldots, x_N)dx_1 \ldots dx_N \tag{12}$$

$$= \left[8A_c + (7A_v - A'_v/2 - A''_v/12)/2^N\right]/15 + E(f)$$

is a composite multidimensional quadrature formula with first- and second-order partial derivative correction terms having degree of precision 5. The truncation error is bounded by

$$|E(f)| \leq w\left[E_6 + 35E_{42} + 280E_{222}\right]/604\,800. \tag{13}$$

PROOF. Let $v = (v_1, \ldots, v_N)$, $v_j = a_j$ or b_j, represent a vertex of R, $c = (c_1, \ldots, c_N)$, $c_j = ½(a_j + b_j)$, the cell centroid, and $m = (m_1, \ldots, m_N)$, $m_j = a_j$ or b_j and $m_i = c_i$ for $i \neq j$, a midpoint of a side. For p = m or v define the sign functionals

$$\sigma_j(p) = \begin{cases} -1 \text{ if } p_j = a_j \\ +1 \text{ otherwise} \end{cases} \tag{14}$$

$$\sigma_{jk}(p) = \sigma_j(p)\sigma_k(p).$$

Then by a linear change of variables, using the notation of (2), and replacing h and h_j in (3) by w and w_j, respectively, one obtains

$$\int_{a_N}^{b_N} \cdots \int_{a_1}^{b_1} f(t_1, \ldots, t_N)dt_1 \ldots dt_N$$

$$= \int_{-h_N}^{h_N} \cdots \int_{-h_1}^{h_1} f\left(\frac{w_1 x_1}{2h_1}, \ldots, \frac{w_N x_N}{2h_N}\right) \frac{w}{h}\, dx_1 \ldots dx_N \tag{15}$$

$$= \frac{8}{15} Q_c + \frac{7}{2^N 15} Q_v - \frac{1}{2^{N+1} 15} Q'_v - \frac{1}{2^{N+2} 45} Q''_v + E(f).$$

The proof follows by applying (15) to each subhyperrectangle of R. Here again, the last term in (13) appears only in the case $N > 2$.

The name MINTOV is also given to (12) since it is the composite formulation of (5). With appropriate interpretation of the centroid and corner nodes and the partial derivative correction terms, MINTOV is a nonproduct N-dimensional generalization of the composite Simpson's formula with end corrections (Lanczos, [12]):

$$\int_a^b f(x)dx = \frac{8h}{15} \sum_{i=1}^{n} f(a+h(i-\tfrac{1}{2})) + \frac{7h}{30} \sum_{i=0}^{n}{}' f(a+ih)$$

$$-\frac{h^2}{60} \left[f'(b) - f'(a)\right] + \frac{b-a}{604800} h^6 f^{(6)}(\xi). \tag{16}$$

The prime on the summation signifies that the weight γ is to be assigned in case the node $a+ih$ is common to γ subintervals. Also, $n=(b-a)/h$, and ξ is some point in $[a,b]$. The number of function evaluations is $2n+3$.

It may also be stated that MINTOV is composite Ewing's formula [5] with partial derivative correction terms. In Section VI, an N-dimensional composite formulation of Ewing's formula is given as D0503.

V. NUMBER OF FUNCTION EVALUATIONS

In this section a partial derivative evaluation is counted the same as a function evaluation. For many integrands it may be necessary to weight the partial derivative evaluations. However, because of the persistence of form property previously noted, the present enumeration technique will be used.

Indeed, for functions such as $\ln(xyz)$ the first-order partials require only about 40% of the time to evaluate the given function, whereas functions similar to $\cos(x)\cos(y)\cos(z)$, $\exp(-xyz)$, $(1+x+y+z)^{-4}$, and even $(1+w)\sin(x)\sin(y)\sin(z)e^{-w}/(xyz)$, $w^2 = x^2+y^2+z^2$, require not more than 5% additional time to evaluate the first- and mixed second-order partials than the original functions.

Now the numbers of function evaluations, ρ, required by the functionals in (11) are

$$\rho(A_c) = \prod_{i=1}^{N} n_i$$

$$\rho(A_v) = \prod_{i=1}^{N} (n_i+1)$$

$$\rho(A_m) = \sum_{j=1}^{N} (n_j+1) \prod_{\substack{i=1 \\ i\neq j}}^{N} n_i$$

$$\rho(A'_v) = 2 \sum_{j=1}^{N} \prod_{\substack{i=1 \\ i\neq j}}^{N} (n_i+1) \tag{17}$$

$$\rho(A'_m) = 2 \sum_{j=1}^{N} \prod_{\substack{i=1 \\ i\neq j}}^{N} n_i$$

$$\rho(A''_v) = 4 \sum_{j<k} \prod_{\substack{i=1 \\ i\neq j,k}}^{N} (n_i+1).$$

Thus, for d-dimensional MINTOV, if $n_i = (b_i - a_i)h_i = n$ for all i, the number of function evaluations is

$$\begin{aligned}\rho &= n^d + (n+1)^d + 2d(n+1)^{d-1} + 2d(d-1)(n+1)^{d-2} \\ &= 2n^d + \sum_{i=0}^{d-1} \left[2(d-i)^2 + 1 \right] \binom{d}{i} n^i.\end{aligned} \tag{18}$$

Hereafter, we refer to n as the number of partitions of R. Note that R is subdivided into n^d subregions.

Let Lyness, Gauss, and Boole represent the composite formulations of C_n:5-5 as listed in Stroud [21] and which is due to Mustard, Lyness, and Blatt [16], the composite product Gauss, and the fifth-order composite product Newton-Cotes formulas, respectively. The number of function evaluations for each rule is given in Table IV. For example, for eight partitions in 4-space, MINTOV, Lyness, Gauss, and Boole require 18 433, 43 425, 331 776, and 1 185 921 function evaluations, respectively.

Table IV

Number of Function Evaluations for Several Fifth-Order Formulas

Formula	ρ
MINTOV	$n^d + (n+1)^{d-2}\ (n+1)^2 + 2d(n+d)$
LYNESS	$(n+1)^d + (2d+1)n^d$
GAUSS	$(3n)^d$
BOOLE	$(4n+1)^d$

It can be shown that for $n > d$, ρ (MINTOV) < ρ (Lyness); equality holds only for $n=d=2$.

Of special interest are the cases d = 2 and 3. In the case d = 2, observe that the composite formulation of the 9-point, degree 5 Lyness cubature formula requires $6n^2 + 2n + 1$ function evaluations, fe. The Radon [18], Albrecht, Collatz [1] 7-point, degree 5 composite formula requires $7n^2$ fe. For brevity, we call it Radon's formula.

As Table IV shows, the 9-point, degree 5 composite product Gauss cubature formula requires $9n^2$ fe, and the 25-point, degree 5 composite product Boole's (Newton-Cotes') rule requires $16n^2 + 8n + 1$ fe.

Tanimoto's [22] fifth-order derivative corrected Simpson's rule requires $4n^2 + 12n + 9$ fe, whereas the fifth-order MINTOV and DH5G5S (see Table VII) rules require only $2n^2 + 6n + 9$ fe and $2n^2 + 10n + 9$ fe, respectively. The composite product formulation of the third order Simpson's rule requires $4n^2 + 4n + 1$ fe.

Table V shows the number of function evaluations these cubature formulas require for various subdivisions. Similar results for the case d = 3 are presented in Table VI. As previously noted, a partial derivative evaluation is counted as one function evaluation.

Table V

Number of Function Evaluations for Various Cubature Formulas Compounded n^2 Times. These are Fifth-Order Formulas Except for Simpson's Rule which is Third-Order

n	MINTOV* $2n^2+6n+9$	DH5G5S* $2n^2+10n+9$	SIMPSON $4n^2+4n+1$	TANIMOTO* $4n^2+12n+9$	LYNESS $6n^2+2n+1$	RADON $7n^2$	GAUSS $9n^2$	BOOLE $16n^2+8n+1$
1	17	21	9	25	9	7	9	25
2	29	37	25	49	29	28	36	81
4	65	81	81	121	105	112	144	289
8	185	217	289	361	401	448	576	1 089
16	617	681	1 089	1 225	1 569	1 792	2 304	4 225
32	2 249	2 377	4 225	4 489	6 209	7 168	9 216	16 641
64	8 585	8 841	16 641	17 161	24 705	28 672	36 864	66 049
100	20 609	21 009	40 401	41 209	60 501	70 000	90 000	160 801

*Partial Derivative Corrected Formulas

Table VI

Number of Function Evaluations for Various 3-Dimensional Quadrature Formulas Repeated n^3 Times

n	MINTOV* $2n^3+9n^2+27n+19$	DH5G5S* $2n^3+15n^2+27n+19$	SH9G5R* $5n^3+18n^2+27n+19$	LYNESS $8n^3+3n^2+3n+1$	SIMPSON $8n^3+12n^2+6n+1$	GAUSS $27n^3$	BOOLE $64n^3+48n^2+12n+1$
1	57	63	69	15	27	27	64
2	125	149	185	83	125	216	729
4	399	495	735	573	729	1 728	4 913
8	1 835	2 219	3 947	4 313	4 913	13 824	35 937
16	10 947	12 483	25 539	33 585	35 937	110 592	274 625
32	75 635	81 779	183 155	265 313	274 625	884 736	2 146 689
64	562 899	587 475	1 386 195	2 109 633	2 146 689	7 077 888	16 974 593
100	2 092 719	2 152 719	5 182 719	8 030 301	8 120 601	27 000 000	64 481 201

*Partial Derivative Corrected Formulas (cf. Table VII)

VI. CONSTRUCTION OF 53 NEW MULTIDIMENSIONAL QUADRATURE RULES WITH PARTIAL DERIVATIVE CORRECTION TERMS AND ERROR ESTIMATES

As in the case of MINTOV, the method of undetermined coefficients is used to construct a number of new formulas. The results are compiled in Table VII; they are n-dimensional generalizations of the cubature formulas given in [10]. Observe that the absolute values of the entries in the Error columns are to be used for the error estimates. The minus signs are a consequence of applying the method of undertermined coefficients and are included for comparison purposes. Also, note that some of the terms become zero for n = 3, 4, and 7.

Entry 26, DC5C5, is MINTOV as given in (12) and (13). For ease of reference, the 2-dimensional formulation will be stated explicitly. To this end let the rectangle $R = [a,b] \times [c,d]$ be partitioned into nm cells each of size $hk = (b-a)(d-c)/nm$. Then

$$\begin{aligned}\int_c^d \int_a^b f(x,y)\,dx\,dy = {} & \frac{8hk}{15} \sum_{j=1}^{m} \sum_{i=1}^{n} f[a+h(i-\tfrac{1}{2}),\ c+k(j-\tfrac{1}{2})] \\ & + \frac{7hk}{60} \sum_{j=0}^{m}{}' \sum_{i=0}^{n}{}' f(a+ih,\ c+jk) \\ & - \frac{h^2k}{120} \sum_{j=0}^{m}{}' \left[f_x(b,\ c+jk) - f_x(a,c+jk)\right] \\ & - \frac{hk^2}{120} \sum_{i=0}^{n}{}' \left[f_y(a+ih,d) - f_y(a+ih,c)\right] \\ & - \frac{h^2k^2}{720} \left[f_{xy}(a,c) - f_{xy}(b,c) + f_{xy}(b,d) - f_{xy}(a,d)\right] \\ & + E(f)\end{aligned} \tag{19}$$

$$|E(f)| \le \frac{(b-a)(d-c)}{604800} \left[(h^6M_1^6 + k^6M_2^6) + 35(h^4k^2M_{12}^{42} + h^2k^4M_{12}^{24})\right] \tag{20}$$

$$\rho\ (\text{MINTOV}) = 2\,(nm) + 3(n+m) + 9. \tag{21}$$

The selection of the formula names assigned to the formulas listed in Table VII was based on the following considerations. The first two symbols were chosen somewhat arbitrarily, whereas a digit was selected for the third symbol to represent the number of function evaluations required for the holistic cubature rule, that is, for $d = 2$ and $n_1 = n_2 = 1$.

Table VII

Multidimensional Quadrature Formulas

No.	Formula	Elements: A_c	A_v	A_m	A'_v	A'_m	A''_v	Error: M_{20}	M_{40}	M_{22}	M_{60}	M_{42}	M^*_{222}
1	MID-POINT EØ101	1						$\frac{1}{24}$					
2	EM143	1				$\frac{1}{24}$			$\frac{-7}{5760}$	$\frac{1}{576}$			
3	ET183	1			$\frac{1}{2^n 12}$				$\frac{-7}{5760}$	$\frac{-5}{576}$			
4	EX183S	1				$\frac{1}{24}$	$\frac{1}{2^n 144}$		$\frac{-7}{5760}$				
5	EC1C3S	1			$\frac{1}{2^n 12}$				$\frac{-7}{5760}$				
6	ES1C3S	1			$\frac{1}{2^n 72}$	$\frac{5}{144}$	$\frac{-5}{2^n 144}$		$\frac{-7}{5760}$				
7	TRAPE-ZOIDAL TØ4Ø1		$\frac{1}{2^n}$					$\frac{-1}{12}$					
8	TM443		$\frac{1}{2^n}$			$\frac{-1}{12}$			$\frac{1}{720}$	$\frac{-1}{72}$			
9	TT483		$\frac{1}{2^n}$		$\frac{-1}{2^n 6}$				$\frac{1}{720}$	$\frac{1}{144}$			
10	TX483S		$\frac{1}{2^n}$			$\frac{-1}{12}$	$\frac{-1}{2^n 18}$		$\frac{1}{720}$				
11	TC4C3S		$\frac{1}{2^n}$		$\frac{-1}{2^n 6}$		$\frac{1}{2^n 36}$		$\frac{1}{720}$				
12	TS4C3S		$\frac{1}{2^n}$		$\frac{-1}{2^n 9}$	$\frac{-1}{36}$			$\frac{1}{720}$				

$^*n > 2$

Table VII (Cont'd)

No.	Formula	Elements						Error					
		A_c	A_v	A_m	A'_v	A'_m	A''_v	M_{20}	M_{40}	M_{22}	M_{60}	M_{42}	M^*_{222}
13	SQUIRE M0401			$\frac{1}{2n}$				$\frac{n-3}{24n}$					
14	MM443			$\frac{1}{2n}$		$\frac{n-3}{24n}$			$\frac{-7n+15}{5760n}$	$\frac{1}{576}$			
15	MT483			$\frac{1}{2n}$	$\frac{n-3}{2^n 12n}$				$\frac{-7n+15}{5760n}$	$\frac{-5n+18}{576n}$			
16	MX483S			$\frac{1}{2n}$		$\frac{n-3}{24n}$	$\frac{1}{2^n 144}$		$\frac{-7n+15}{5760n}$				
17	MC4C3S			$\frac{1}{2n}$	$\frac{n-3}{2^n 12n}$				$\frac{-7n+15}{5760n}$				
18	MS4C3S			$\frac{1}{2n}$	$\frac{1}{2^n 72}$	$\frac{5n-18}{144n}$	$\frac{-5n+18}{2^n 144n}$		$\frac{-7n+15}{5760n}$				
19	EWING D0503	$\frac{2}{3}$	$\frac{1}{2^n 3}$						$\frac{-1}{2880}$	$\frac{-1}{288}$			
20	DF543S	$\frac{2}{3}$	$\frac{1}{2^n 3}$				$\frac{-1}{2^n 72}$		$\frac{-1}{2880}$				
21	DM543A	$\frac{8}{9}$	$\frac{1}{2^n 9}$			$\frac{1}{36}$			$\frac{-1}{1080}$				
22	DM543B	$\frac{8}{15}$	$\frac{7}{2^n 15}$			$\frac{-1}{60}$				$\frac{-1}{180}$			
23	DT583A	$\frac{4}{9}$	$\frac{5}{2^n 9}$		$\frac{-1}{2^n 18}$				$\frac{1}{4320}$				
24	DT583B	$\frac{8}{15}$	$\frac{7}{2^n 15}$		$\frac{-1}{2^n 30}$					$\frac{-1}{720}$			
25	DX585	$\frac{8}{15}$	$\frac{7}{2^n 15}$			$\frac{-1}{60}$	$\frac{-1}{2^n 45}$				$\frac{1}{604800}$	$\frac{7}{69120}$	$\frac{43}{34560}$
26	DC5C5	$\frac{8}{15}$	$\frac{7}{2^n 15}$		$\frac{-1}{2^n 30}$		$\frac{-1}{2^n 180}$				$\frac{1}{604800}$	$\frac{1}{17280}$	$\frac{1}{2160}$
27	DS5C5	$\frac{8}{15}$	$\frac{7}{2^n 15}$		$\frac{-2}{2^n 45}$	$\frac{1}{180}$					$\frac{1}{604800}$	$\frac{1}{23040}$	$\frac{7}{34560}$
28	DH5G5R*	$\frac{8}{15}$	$\frac{7}{2^n 15}$		$\frac{-43}{2^n 810}$	$\frac{4}{405}$	$\frac{7}{2^n 1620}$				$\frac{1}{604800}$	$\frac{1}{31104}$	
29	DH5G5S	$\frac{8}{15}$	$\frac{7}{2^n 15}$		$\frac{-7}{2^n 90}$	$\frac{1}{45}$	$\frac{1}{2^n 60}$				$\frac{1}{604800}$		$\frac{-1}{1728}$

* $n > 2$

Table VII (Cont'd)

No.	Formula	Elements						Error					
		A_c	A_v	A_m	A'_v	A'_m	A''_v	M_{20}	M_{40}	M_{22}	M_{60}	M_{42}	M^*_{222}
30	TYLER XØ5Ø3	$\frac{-n+3}{3}$		$\frac{1}{6}$					$\frac{-1}{2880}$	$\frac{1}{576}$			
31	XF543S	$\frac{-n+3}{3}$		$\frac{1}{6}$			$\frac{1}{2^n 144}$		$\frac{-1}{2880}$				
32	XM543T	$\frac{-7n+15}{15}$		$\frac{7}{30}$		$\frac{-1}{60}$				$\frac{1}{576}$			
33	XT583A	$\frac{-5n+18}{18}$		$\frac{5}{36}$	$\frac{1}{2^n 72}$				$\frac{-17}{34560}$				
34	XT583B	$\frac{-7n+15}{15}$		$\frac{7}{30}$	$\frac{-1}{2^n 30}$					$\frac{17}{2880}$			
35	XX585	$\frac{-7n+15}{15}$		$\frac{7}{30}$		$\frac{-1}{60}$	$\frac{1}{2^n 144}$				$\frac{1}{604800}$	$\frac{-7}{138240}$	$\frac{-1}{1728}$
36	XC5C5	$\frac{-7n+15}{15}$		$\frac{7}{30}$	$\frac{-1}{2^n 30}$		$\frac{17}{2^n 720}$				$\frac{1}{604800}$	$\frac{-13}{138240}$	$\frac{-47}{34560}$
37	XS5C5	$\frac{-7n+15}{15}$		$\frac{7}{30}$	$\frac{1}{2^n 72}$	$\frac{-17}{720}$					$\frac{1}{604800}$	$\frac{-1}{30720}$	$\frac{-7}{27648}$
38	XH5G5R*	$\frac{-7n+15}{15}$		$\frac{7}{30}$	$\frac{2}{2^n 81}$	$\frac{-47}{1620}$	$\frac{-7}{2^n 1296}$				$\frac{1}{604800}$	$\frac{67}{1244160}$	
39	XH5G5S	$\frac{-7n+15}{15}$		$\frac{7}{30}$	$\frac{7}{2^n 180}$	$\frac{-13}{360}$	$\frac{-1}{2^n 80}$				$\frac{1}{604800}$		$\frac{23}{69120}$
40	MILLER OØ8Ø3		$\frac{n-3}{3(n-1)2^n}$	$\frac{1}{3(n-1)}$					$\frac{-1}{2880}$	$\frac{-n+4}{288(n-1)}$			
41	OF843S		$\frac{n-3}{3(n-1)2^n}$	$\frac{1}{3(n-1)}$			$\frac{-n+4}{72(n-1)2^n}$		$\frac{-1}{2880}$				
42	OM843A		$\frac{1}{2^n 9}$	$\frac{4}{9n}$		$\frac{n-4}{36n}$			$\frac{-2n+5}{2160n}$				
43	OM843B		$\frac{7n-15}{15(n-1)2^n}$	$\frac{4}{15(n-1)}$		$\frac{-1}{60}$				$\frac{-2n+5}{306(n-1)}$			
44	OT883A*		$\frac{5n-18}{9(n-2)2^n}$	$\frac{2}{9(n-2)}$	$\frac{-n+4}{18(n-2)2^n}$				$\frac{n-7}{4320(n-2)}$				
45	OT883B		$\frac{7n-15}{15(n-1)2^n}$	$\frac{4}{15(n-1)}$	$\frac{-1}{2^n 30}$					$\frac{-n+7}{720(n-1)}$			
46	OX885		$\frac{7n-15}{15(n-1)2^n}$	$\frac{4}{15(n-1)}$		$\frac{-1}{60}$	$\frac{-2n+5}{90(n-1)2^n}$				$\frac{1}{604800}$	$\frac{7n-19}{69120(n-1)}$	$\frac{387n-1035}{311040(n-1)}$
47	OC8C5		$\frac{7n-15}{15(n-1)2^n}$	$\frac{4}{15(n-1)}$	$\frac{-1}{2^n 30}$		$\frac{-n+7}{180(n-1)2^n}$				$\frac{1}{604800}$	$\frac{n-4}{17280(n-1)}$	$\frac{2n-11}{4320(n-1)}$
48	OS8C5		$\frac{7n-15}{15(n-1)2^n}$	$\frac{4}{15(n-1)}$	$\frac{-2n+5}{45(n-1)2^n}$	$\frac{n-7}{180(n-1)}$					$\frac{1}{604800}$	$\frac{-n+3}{23040(n-1)}$	$\frac{7n-25}{34560(n-1)}$
49	OH8G5R*		$\frac{7n-15}{15(n-1)2^n}$	$\frac{4}{15(n-1)}$	$\frac{-43n+115}{810(n-1)2^n}$	$\frac{2n-11}{405(n-1)}$	$\frac{7n-25}{1620(n-1)2^n}$				$\frac{1}{604800}$	$\frac{5n-14}{155520(n-1)}$	
50	OH8G5S		$\frac{7n-15}{15(n-1)2^n}$	$\frac{4}{15(n-1)}$	$\frac{-7n+19}{90(n-1)2^n}$	$\frac{n-4}{45(n-1)}$	$\frac{n-3}{60(n-1)2^n}$				$\frac{1}{604800}$		$\frac{-5n+14}{8640(n-1)}$

* $n > 2$

Table VII (Cont'd)

No.	Formula	Elements						Error					
		A_c	A_v	A_m	A'_v	A'_m	A''_v	M_{20}	M_{40}	M_{22}	M_{60}	M_{42}	M^*_{222}
51	SIMPSON (n=2) SØ9Ø3S	$\frac{-2(n-4)}{9}$	$\frac{1}{2^n 9}$	$\frac{1}{9}$					$\frac{-1}{2800}$				
52	SM945	$\frac{-8(2n-5)}{45}$	$\frac{1}{2^n 9}$	$\frac{8}{45}$		$\frac{-1}{60}$					$\frac{1}{604800}$	$\frac{-1}{69120}$	$\frac{-1}{6912}$
53	ST985	$\frac{-4(n-7)}{45}$	$\frac{17}{2^n 45}$	$\frac{2}{45}$	$\frac{-1}{2^n 30}$						$\frac{1}{604800}$	$\frac{1}{34560}$	$\frac{1}{23040}$
54	SX985R*	$\frac{-43n+115}{135}$	$\frac{4}{2^n 27}$	$\frac{43}{270}$		$\frac{-1}{60}$	$\frac{-1}{2^n 432}$				$\frac{1}{604800}$	$\frac{-1}{165888}$	
55	SX985S	$\frac{-2(7n-19)}{45}$	$\frac{7}{2^n 45}$	$\frac{7}{45}$		$\frac{-1}{60}$	$\frac{-1}{2^n 360}$				$\frac{1}{604800}$		$\frac{1}{34560}$
56	SC9C5R*	$\frac{-8(2n-11)}{135}$	$\frac{47}{2^n 135}$	$\frac{8}{135}$	$\frac{-1}{2^n 30}$		$\frac{1}{2^n 540}$				$\frac{1}{604800}$	$\frac{1}{17280}$	
57	SC9C5S	$\frac{-8(n-4)}{45}$	$\frac{13}{2^n 45}$	$\frac{4}{45}$	$\frac{-1}{2^n 30}$		$\frac{1}{2^n 180}$				$\frac{1}{604800}$		$\frac{-1}{4320}$
58	SS9C5R*	$\frac{-4(7n-25)}{135}$	$\frac{7}{2^n 27}$	$\frac{14}{135}$	$\frac{-1}{2^n 54}$	$\frac{-1}{135}$					$\frac{1}{604800}$	$\frac{1}{103680}$	
59	SS9C5S	$\frac{-4(n-3)}{15}$	$\frac{1}{2^n 5}$	$\frac{2}{15}$	$\frac{-1}{2^n 90}$	$\frac{-1}{90}$					$\frac{1}{604800}$		$\frac{-1}{17280}$
60	SH9G5R*	$\frac{-8(5n-14)}{135}$	$\frac{23}{2^n 135}$	$\frac{4}{27}$	$\frac{-1}{2^n 270}$	$\frac{-2}{135}$	$\frac{-1}{2^n 540}$				$\frac{1}{604800}$		

*n > 2

The fourth symbol represents the number of partial derivative evaluations required for the holistic cubature rule. The fifth digit is the degree of precision of the formula. The presence of a sixth symbol signifies that the method of undetermined coefficients led to more equations than unknowns. The letters A and B are used to indicate two successful combinations, whereas an R, S, or T indicates at least one unsuccessful combination.

For completeness, formulas 1 and 7, the composite formulations of the midpoint [9] and trapezoidal rules, respectively, have been included. Formula 51 is equivalent to the composite Simpson's rule for N=2. The holistic representation (i.e., $n_\alpha = 1$ for all α) for formulas 13, 19, 30, and 40 were investigated by Squire [20], Ewing [5], Tyler [23], and Miller [15], respectively. Formula 30 was apparently discovered independently by Bickley [2] and Tyler [23]. We will follow Stroud [21] and call it Tyler's rule. Thus, except for formulas 1, 7, 13, 19, 30, 40, and 51, the remaining 53 multidimensional quadrature formulas are new.

In the two-dimensional case, it is interesting to compare DF543S with Simpson's cubature rule, S0903S, because both are third-order formulas and both have the same error bounds; however, the former requires approximately half as many function evaluations as Simpson's rule. Specifically, the formulas require $2(n_1 n_2) + (n_1 + n_2) + 5$ and $4(n_1 n_2) + 2(n_1 + n_2) + 1$ function evaluations, respectively.

DF543S is a combined trapezoidal-midpoint or Ewing rule [5] with boundary correction terms. This cubature rule requires mixed second-order partial derivatives evaluated only at the corners of the rectangular domain of integration R.

Two formulas, XF543S and OF893S, which share this property with DF543S also have the same error bound as Simpson's rule. There may be applications where the cubature rule DF543S should be considered as a viable alternative to Simpson's rule.

Finally, we note that numerical results for double integrals indicate that EM143 is competitive with Simpson's rule since it requires only $(n_1 n_2) + 2(n_1 + n_2)$ function evaluations as compared with $4(n_1 n_2) + 2(n_1 + n_2) + 1$ for Simpson.

VII. NUMERICAL RESULTS

Example 1

$$\int_0^1 \int_0^1 \frac{dxdy}{1+(xy)^2} = \int_0^{\frac{\pi}{2}} \int_0^{\frac{\pi}{2}} \frac{dxdy}{2(1+\cos(x)\cos(y))} = \int_0^1 \frac{\tan^{-1}(x)}{x} dx \tag{22}$$

$$= 0.915\ 965\ 594\ 177.$$

Taking $f(x,y) = (1+x^2y^2)^{-1}$ and $h=k=\frac{1}{2}$ in (19) we obtain

$$I(f) \simeq \frac{8}{15} \frac{1}{4} \left[\frac{256}{257} + 2\left(\frac{256}{265}\right) + \frac{256}{337}\right]$$

$$+ \frac{7}{60} \frac{1}{4} \left[1 + 2(1) + \frac{1}{2} + 2(2)(1) + 2(2)\frac{4}{5} + 4\frac{16}{17}\right]$$

$$- \frac{1}{120} \frac{1}{8} \left[-\frac{1}{2} - 2\left(\frac{8}{25}\right)\right] (2) \tag{23}$$

$$= 0.491\ 710\ 445 + 0.421\ 887\ 255 + 0.002\ 375\ 000$$

$$= 0.915\ 972\ 700\ 0.$$

The error is 0.000 007 106 8. Here $f_x = -2xy^2(1+x^2y^2)^{-2}$ and $f_{xy} = 4xy(x^2y^2-1)(1+x^2y^2)^{-2}$. The first-order partial derivatives f_x and f_y vanish on the axes while the second-order mixed partial derivative f_{xy} vanishes at the corners as well as on the axes.

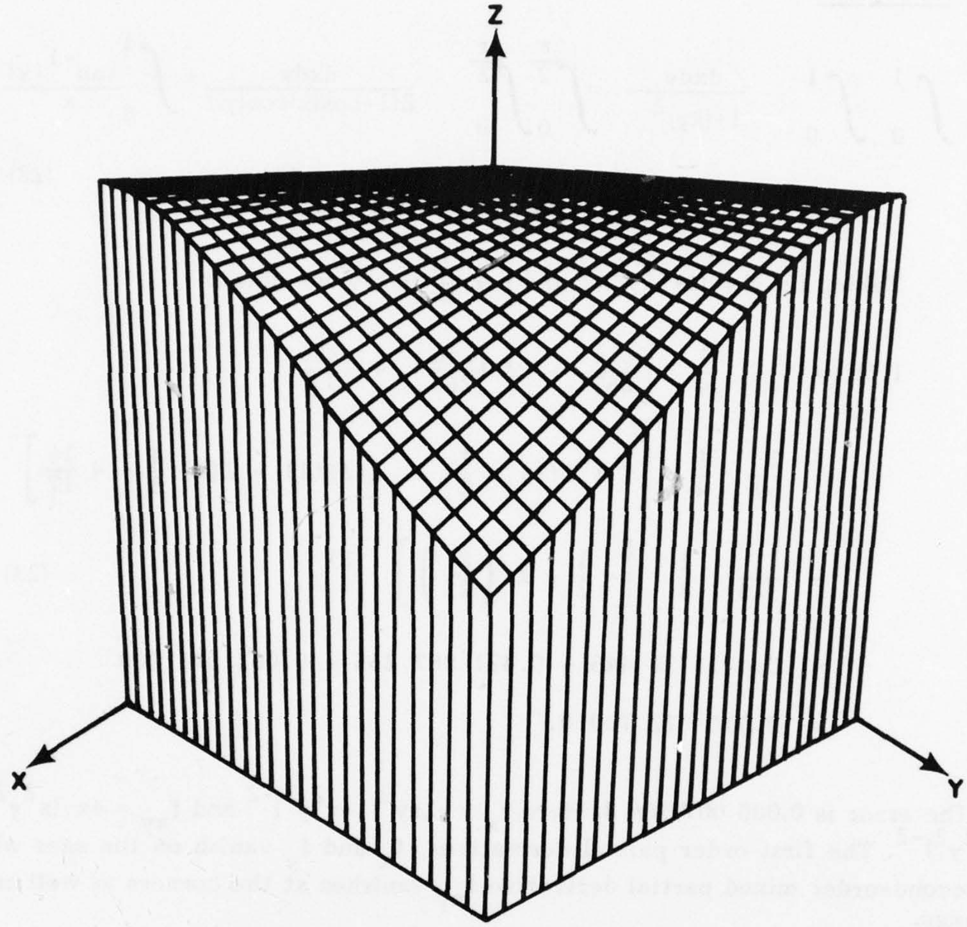


Figure 4
Graph of $z = (1+x^2y^2)^{-1}$ on $\left[0,1\right]^2$

Numerical results are presented in Table VIII. As before, ρ represents the number of function (and/or partial derivative) evaluations.

Table VIII

$$\int_0^1 \int_0^1 \frac{dxdy}{1+x^2y^2} = 0.915\ 965\ 594\ 177$$

No.*	Formula	$h = k = \frac{1}{5}$ (n=m=5)		$h = k = \frac{1}{10}$ (n=m=10)		Order
		ρ	Error	ρ	Error	
	MIDPOINT					
1	EØ1Ø	25	-9.52-4†	100	-2.38-4	1
2	EM143	45	-1.11-6	140	-6.97-8	3
3	ET183	49	-1.15-6	144	-7.04-8	3
4	EX183S	49	-1.11-6	144	-6.97-8	3
5	EC1C3S	53	-1.15-6	148	-7.04-8	3
6	ES1C3S	69	-1.11-6	184	-6.98-8	3
	TRAPE-ZOIDAL					
7	TØ4Ø1	36	1.90-3	121	4.76-4	1
8	TM443	56	1.18-6	161	7.84-8	3
9	TT483	60	1.27-6	165	7.97-8	3
10	TX483S	60	1.18-6	165	7.84-8	3
11	TC4C3S	64	1.27-6	169	7.97-8	3
12	TS4C3S	80	1.24-6	205	7.93-8	3
	SQUIRE					
13	MØ4Ø1	60	3.76-4	220	1.19-4	1
14	MM443	80	1.01-7	260	5.32-9	3
15	MT483	84	1.22-7	264	5.64-9	3
16	MX483S	84	1.01-7	264	5.32-9	3
17	MC4C3S	88	1.22-7	268	5.64-9	3
18	MS4C3S	104	9.39-8	304	5.21-9	3
	EWING					
19	DØ5Ø3	61	-3.44-7	221	-2.04-8	3
20	DF543S	65	-3.44-7	225	-2.04-8	3
21	DM543A	81	-8.53-7	261	-5.33-8	3
22	DM543B	81	-3.88-8	261	-6.01-10	3
23	DT583A	85	1.93-7	265	1.30-8	3
24	DT583B	85	-2.20-8	265	-3.39-10	3
25	DX585	85	-3.88-8	265	-6.01-10	5
26	MINTOV	89	-2.20-8	269	-3.39-10	5
27	DS5C5	105	-1.64-8	305	-2.52-10	5
29	DH5G5S	109	4.31-10	309	8.61-12	5

*See Table VII

†$-9.52\text{-}4 = -9.52 \times 10^{-4}$

Table VIII (Cont'd)

		$h = k = \frac{1}{5}$ (n=m=5)		$h = k = \frac{1}{10}$ (n=m=10)		
No.	Formula	ρ	Error	ρ	Error	Order
	TYLER					
30	XØ5Ø3	85	-3.02-7	320	-1.97-8	3
31	XF543S	89	-3.02-7	324	-1.97-8	3
32	XM543T	105	2.04-8	360	3.14-10	3
33	XT583A	109	-4.43-7	364	-2.81-8	3
34	XT583B	109	3.72-8	364	5.75-10	3
35	XX585	109	2.04-8	364	3.14-10	5
36	XC5C5	113	3.72-8	368	5.75-10	5
37	XS5C5	129	1.34-8	404	2.06-10	5
39	XH5G5S	133	7.31-10	408	9.76-12	5
	MILLER					
40	OØ8Ø3	96	-2.60-7	341	-1.90-8	3
41	OF843S	100	-2.60-7	345	-1.90-8	3
42	OM843A	116	2.21-7	381	1.34-8	3
43	OM843B	116	2.88-8	381	4.45-10	3
45	OT883B	120	4.56-8	385	7.06-10	3
46	OX885	120	2.88-8	385	4.45-10	5
47	OC8C5	124	4.56-8	389	7.06-10	5
48	OS8C5	140	1.76-8	425	2.71-10	5
50	OH8G5S	144	7.74-10	429	9.92-12	5
	SIMPSON					
51	SØ9Ø3S	121	-3.16-7	441	-1.99-8	3
52	SM945	141	6.27-9	481	9.65-11	5
53	ST985	145	-1.07-8	485	-1.65-10	5
55	SX985S	145	6.31-10	485	9.37-12	5
57	SC9C5S	149	5.46-10	489	9.04-12	5
59	SS9C5S	165	6.03-10	525	9.26-12	5
	TANIMOTO	169	5.91-10	529	9.22-12	5
	LYNESS	161	5.66-9	621	8.70-11	5
	RADON	175	-1.84-9	700	-2.81-11	5
	GAUSS	225	1.78-10	900	2.83-12	5
	BOOLE	441	-1.85-10	1681	-2.77.12	5

These examples were run on the U.S. NAVAIRTESTCEN's Real-Time Telemetry Processing System Xerox Sigma 9 computer using the CPR version E00 operating system and FORTRAN IV in double precision with 15+ significant decimal digits.

Example 2 (Stroud, [21])

$$\int_{-1}^{1} \int_{-1}^{1} \sqrt{3+x+y}\ dxdy = \frac{4}{15} (1 - 18\sqrt{3} + 25\sqrt{5}) \qquad (24)$$

$$= 6.859\ 942\ 640\ 334\ 65.$$

Results for $h=k=\frac{1}{3}$ are presented in Table IX. For this example, the computed error bounds provide reasonably close estimates to the actual errors.

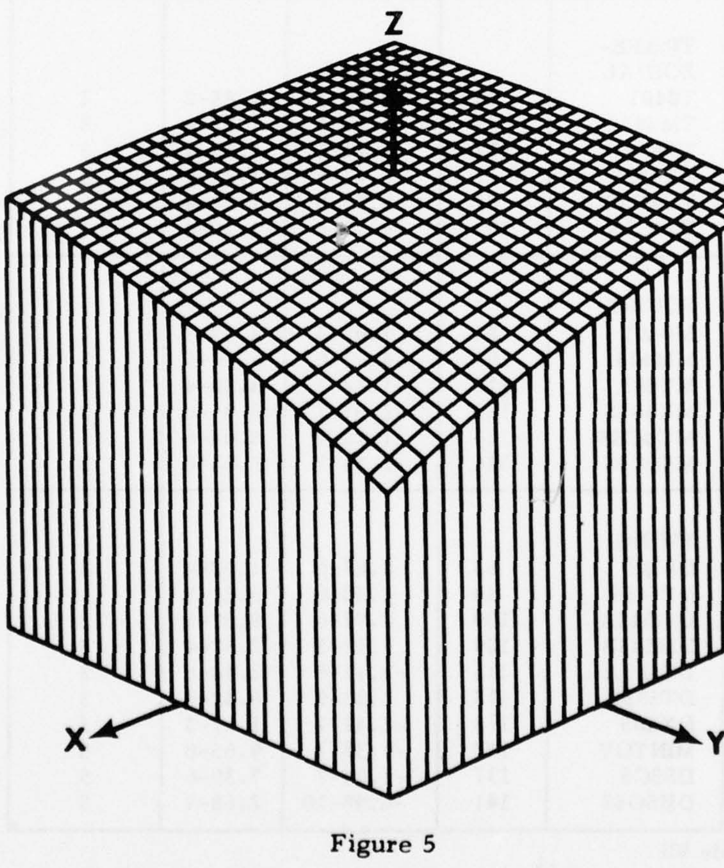


Figure 5

Graph of $z = \sqrt{3+x+y}$ on $[-1,1]^2$

Table IX

$$\int_{-1}^{1}\int_{-1}^{1}\sqrt{3+x+y}\;dxdy = 6.859\ 942\ 640\ 334\ 65$$

No.*	Formula	$h = k = \frac{1}{3}$ (n = m = 6)			Order
		ρ	Error	Error Bound	
	MIDPOINT				
1	EØ1Ø1	36	-2.10-3†	9.26-3	1
2	EM143	60	1.44-6	1.93-4	3
3	ET183	64	2.38-5	5.14-4	3
4	EX183S	64	5.21-6	1.13-4	3
5	EC1C3S	68	4.96-6	1.13-4	3
6	ES1C3S	88	5.17-6	1.13-4	3
	TRAPE-ZOIDAL				
7	TØ4Ø1	49	4.23-3	1.85-2	1
8	TM443	73	2.73-5	7.72-4	3
9	TT483	77	-2.11-5	4.50-4	3
10	TX483S	77	-6.47-6	1.29-4	3
11	TC4C3S	81	-5.96-6	1.29-4	3
12	TS4C3S	101	-6.13-6	1.29-4	3
	SQUIRE				
13	MØ4Ø1	84	1.05-3	4.63-3	1
14	MM443	108	-4.03-6	8.84-5	3
15	MT483	112	-1.52-5	3.30-4	3
16	MX483S	112	-2.51-7	8.04-6	3
17	MC4C3S	116	-1.22-7	8.04-6	3
18	MS4C3S	136	-2.94-7	8.04-6	3
	EWING				
19	DØ5Ø3	85	8.87-6	1.93-4	3
20	DF543S	89	1.32-6	3.22-5	3
21	DM543A	109	3.91-6	8.57-5	3
22	DM543B	109	1.18-5	2.57-4	3
23	DT583A	113	-1.11-6	2.14-5	3
24	DT583B	113	2.88-6	6.43-5	3
25	DX585	113	-2.41-7	1.67-5	3
26	MINTOV	117	-1.38-7	9.65-6	5
27	DS5C5	137	-1.04-7	7.30-6	5
29	DH5G5S	141	-6.98-10	2.68-7	5

*See Table VII

†$-2.10-3 = 2.10 \times 10^{-3}$

Table IX (Cont'd)

No.	Formula	$h = k = \frac{1}{3}$ (n = m = 6) ρ	Error	Error Bound	Order
	TYLER				
30	XØ5Ø3	120	-2.21-6	1.13-4	3
31	XF543S	124	1.57-6	3.22-5	3
32	XM543T	144	-3.66-6	8.04-5	3
33	XT583A	148	2.13-6	4.55-5	3
34	XT583B	148	-1.26-5	2.73-4	3
35	XX585	148	1.13-7	8.47-6	5
36	XC5C5	152	2.16-7	1.55-5	5
37	XS5C5	172	7.05-8	5.54-6	5
39	XH5G5S	176	-6.66-9	2.68-7	5
	MILLER				
40	OØ8Ø3	133	-1.33-5	3.54-4	3
41	OF843S	137	1.83-6	3.22-5	3
42	OM843A	157	-9.42-7	2.14-5	3
43	OM843B	157	-5.88-6	1.29-4	3
45	OT883B	161	-1.48-5	3.22-4	3
46	OX885	161	1.64-7	1.20-5	5
47	OC8C5	165	2.67-7	1.90-5	5
48	OS8C5	185	9.53-8	7.30-6	5
50	OH8G5S	189	-7.51-9	2.68-7	5
	SIMPSON				
51	SØ9Ø3S	169	1.49-6	3.22-5	3
52	SM945	193	2.90-8	2.61-6	5
53	ST985	197	-7.04-8	4.96-6	5
55	SX985S	197	-4.67-9	2.68-7	5
57	SC9C5S	201	-2.97-9	2.68-7	5
59	SS9C5S	221	-4.10-9	2.68-7	5
	TANIMOTO	225	-3.88.9	-	5
	LYNESS	229	3.28-8	-	5
	RADON	252	-1.12-8	-	5
	GAUSS	324	-1.16-9	-	5
	BOOLE	625	1.21-9	-	5

Example 3

$$\int_0^{\frac{\pi}{2}} \int_0^{\frac{\pi}{2}} \int_0^{\frac{\pi}{2}} \frac{1+w}{xyz} \sin(x)\sin(y)\sin(z)\, e^{-w}\, dxdydz \tag{25}$$

$$= 1.531\ 670\ 226\ 93,$$

where $w^2 = x^2+y^2+z^2$. The first-order partial derivative with respect to x is

$$f_x(x,y,z) = \left[(1+w)\cos(x) - (1+w+x^2)\frac{\sin(x)}{x}\right] \frac{\sin(y)\sin(z)e^{-w}}{xyz} \tag{26}$$

and the mixed second-order partial with respect to x and y is

$$f_{xy}(x,y,z) = \left[(1+w)\cos(x)\cos(y) + \frac{w+w^2+w(x^2+y^2) + x^2y^2}{wyz} \sin(x)\sin(y)\right.$$

$$\left. - \frac{1+w+x^2}{x} \sin(x)\cos(y) - \frac{1+w+y^2}{y} \cos(x)\sin(y)\right] \frac{\sin(z)e^{-w}}{xyz} \tag{27}$$

The results of applying each of the formulas of Table VII to the integral in (24) with $n_i = 8 (h_i = \pi/16)$ are presented in Table X. Note that for triple integrals, the following formulas listed in Table VII coincide: 13=14=15; 16=17; 31=41; and 48=50=59.

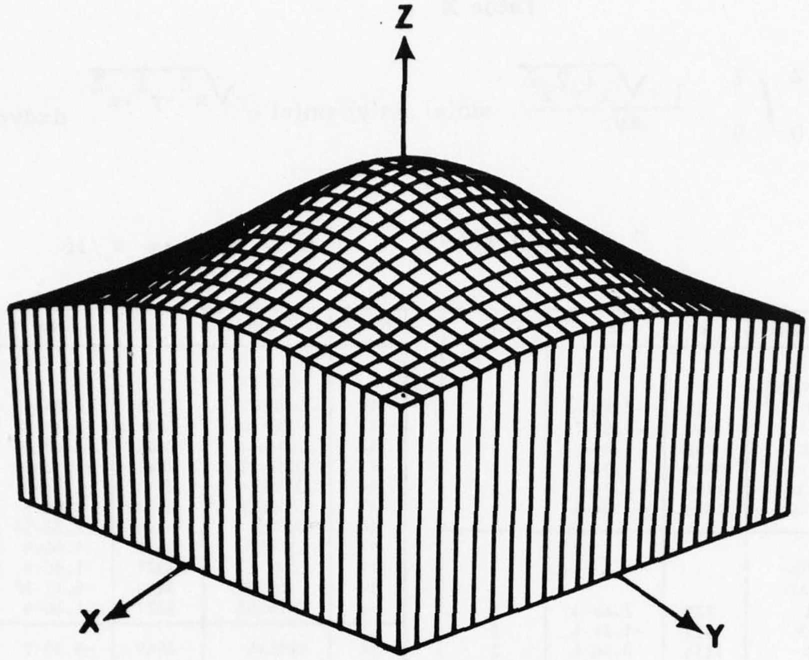


Figure 6

Graph of $z = \frac{1+\sqrt{x^2+y^2}}{xy} \sin(x)\sin(y)e^{-\sqrt{x^2+y^2}}$ on $\left[\frac{-\pi}{2}, \frac{\pi}{2}\right]^2$

Table X

$$\int_0^2 \int_0^2 \int_0^2 \frac{1+\sqrt{x^2y^2z^2}}{xyz} \sin(x)\sin(y)\sin(z)\, e^{-\sqrt{x^2+y^2+z^2}}\, dxdydz$$

$$= 1.531\ 670\ 22693, \qquad n_i = 8,\ h_i = \pi/16$$

No.*	Formula	ρ	Error	Order
	MIDPOINT			
1	EØ1Ø1	512	-2.85-3†	1
2	EM143	896	-1.57-7	3
3	ET183	998	-1.09-5	3
4	EX183S	1004	-1.94-6	3
5	EC1C3S	1106	-1.95-6	3
6	ES1C3S	1382	-1.94-6	3
	TRAPE-ZOIDAL			
7	TØ4Ø1	729	5.68-3	1
8	TM443	1113	-1.21-5	3
9	TT483	1215	9.30-6	3
10	TX483S	1221	2.15-6	3
11	TC4C3S	1323	2.19-6	3
12	TS4C3S	1599	2.17-6	3
	SQUIRE			
13	MØ4Ø1	1728	1.24-6	1
14	MM443	1728	1.24-6	3
15	MT483	1728	1.24-6	3
16	MX483S	1836	-5.39-7	3
17	MC4C3S	1836	-5.39-7	3
18	MS4C3S	2598	-5.42-7	3
	EWING			
19	DØ5Ø3	1241	-4.13-6	3
20	DF543S	1349	-5.73-7	3
21	DM543A	1625	-1.48-6	3
22	DM543B	1625	-5.72-6	3
23	DT583A	1727	3.46-7	3
24	DT583B	1727	-1.44-6	3
25	DX585	1733	-2.77-8	3
26	DC5C5	1835	-2.13-8	5
27	DS5C5	2111	-1.92-8	5
28	DH5G5R	2219	-1.75-8	5
29	DH5G5S	2219	-1.28-8	5
	TYLER			
30	XØ5Ø3	1728	1.24-6	3
31	XF543S	1836	-5.39-7	3
32	XM543T	2624	1.79-6	3
33	XT583A	2726	-7.75-7	3
34	XT583B	2726	6.07-6	3
35	XX585	2732	1.95-8	5
36	XC5C5	2834	2.59-8	5
37	XS5C5	3110	1.68-8	5
38	XH5G5R	3218	1.48-8	5
39	XH5G5S	3218	1.21-8	5

No.*	Formula	ρ	Error	Order
	MILLER			
40	OØ8Ø3	1728	1.24-6	3
41	OF843S	1836	-5.39-7	3
42	OM843A	2841	-2.40-7	3
43	OM843B	2841	-1.42-6	3
44	OT883A	2943	-1.45-6	3
45	OT883B	2943	2.85-6	3
46	OX885	2949	-7.28-10	5
47	OC8C5	3051	5.66-9	5
48	OS8C5	3327	1.40-9	5
49	OH8G5R	3435	9.27-10	5
50	OH8G5S	3327	1.40-9	5
51	SØ9Ø3S	2969	-5.50-7	3
52	SM945	3353	8.27-9	5
53	ST985	3455	-1.23-8	5
54	SX985R	3461	4.52-9	5
55	SX985S	3461	3.77-9	5
56	SC9C5R	3563	-9.33-9	5
57	SC9C5S	3563	-3.34-9	5
58	SS9C5R	3839	-3.18-9	5
59	SS9C5S	3327	1.40-9	5
60	SH9G5R	3947	2.98-9	5
	LYNESS	4313	4.94-9	5
	GAUSS	13824	1.08-9	5
	SIMPSON	4913	-5.49-7	3

*See Table VII

†$-2.85\text{-}3 = -2.85 \times 10^{-3}$

VIII. CONCLUSIONS

We have investigated the problem of enhancing the accuracy of conventional formulas for evaluating multiple integrals numerically over n-dimensional rectangles by the addition of first- and/or mixed second-order partial derivative correction terms evaluated on the boundary of the domain of integration. Efficiency was achieved by the judicious application of the alternating sign property. In Table VII, 53 new multidimensional quadrature formulas with boundary partial derivative correction terms were given. Numerical results for double and triple integrals indicate the new formulas are both accurate and efficient.

In applications where first- and perhaps mixed second-order partial derivatives of the integrand are readily computed, the new formulas should be preferred to traditional rules. Specifically, some of the new formulas may be useful in finite element applications.

Future studies should consider the addition of weight functions, more general domains of integration, higher-order partial derivative correction terms, additional and arbitrary node locations, and the use of Gregory-type difference correction terms in place of the first-order partial derivative correction terms.

Finally, we conjecture that formula EM143 (Table VII) may be the first of a class of Gaussian-type partial derivative corrected multidimensional quadrature formulas.

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